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Abstract

It is shown that the expansion in density of spin deviations for the Heisenberg antiferromagnet at low temperatures leads to a $1/z$ expansion for the free energy. In contrast to the $1/S$ expansion, the kinematic properties of spin operators are realized within each order of the expansion. The spin-wave energy at long wavelength is also calculated.

Disciplines

Physics

1/z EXPANSION FOR THE HEISENBERG ANTIFERROMAGNET AT LOW TEMPERATURES*

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It is shown that the expansion in density of spin deviations for the Heisenberg antiferromagnet at low temperatures leads to a 1/z expansion for the free energy. In contrast to the 1/S expansion, the kinematic properties of spin operators are realized within each order of the expansion. The spin-wave energy at long wavelength is also calculated.

The purpose of this Letter is to describe a method whereby contributions to the thermodynamic properties of the Heisenberg antiferromagnet at low temperatures can be classified according to a parameter which is roughly equivalent to 1/z, where z is the number of nearest neighbors. One advantage of the present formulation is that, in contrast to the usual 1/S expansion,¹ the kinematics of spin operators are preserved in each order. As a result we obtain for the first time an excitation spectrum including the effects of spin-wave interactions and anisotropy which has no gap for spin 1/2. Secondly, our method of obtaining the 1/z expansion is sufficiently simple algebraically to enable us to quote several new results, some involving infinite order perturbation theory.

We consider the Hamiltonian

$$H = 2J \sum_{\langle ij \rangle} S_i S_j - D \sum_i S_{iz}^2, \quad (1)$$

where the first sum is over nearest-neighbor pairs in a d-dimensional cubic lattice. Using the Dyson-Maleev transformation^{2,3} to boson operators we write this as

$$H = E_0 + H_0 + V, \quad (2)$$

with

$$E_0 = -2JzS^2N - 2NDS^2, \quad (3a)$$

$$H_0 = (H_E + H_A) \left(\sum_k a_k^\dagger a_k + b_k^\dagger b_k + \xi \gamma_k a_k^\dagger b_k^\dagger + \xi \gamma_k a_k b_{-k} \right), \quad (3b)$$

$$V = -N^{-1} \sum_{1234} \delta_k (1 + 2 - 3 - 4) [H_{E/S} (a_1^\dagger b_2^\dagger a_3 b_4 \gamma_{2-4} + \frac{1}{2} a_1^\dagger b_{-2}^\dagger a_3 a_4 \gamma_{2-4} + \frac{1}{2} a_1^\dagger b_2^\dagger b_{-3}^\dagger b_{-4} \gamma_{3+4-2}) \\ + D (a_1^\dagger a_2^\dagger a_3 a_4 + b_1^\dagger b_2^\dagger b_3 b_4)] \quad (3c)$$

in the usual notation⁴ with $H_E = 2JzS$, $H_A = D(2S - 1)$, and $\xi = H_E/(H_E + H_A)$. Note that for spin 1/2, $S_{iz}^2 = 1/4$, so that perturbative contributions to the free energy should be independent of D and the excitation spectrum should exhibit no gap. Our results suggest that these statements are true order by order in the 1/z expansion.

One is led to such an expansion from rather general considerations. For the ferromagnet^{2,5} one obtains an expansion in powers of the density, $\rho_F(T)$, of spin waves, where $\rho_F(T) \sim T^{3/2}$. One might also expect to be able to make a similar expansion for an antiferromagnet, except that here $\rho(T) \sim \rho(0) + \rho_1(T)$. Since for $D=0$ long-wavelength spin waves interact only very weakly, $\rho_F(T)$ and $\rho_1(T)$ are actually replaced by $\rho_F^{\text{eff}}(T) = T\rho_F(T)$ and $\rho_1^{\text{eff}}(T) = T^2\rho_1(T)$, respectively.

Thus we expect to expand the free energy as

$$F = F_0 + \sum_{n+m \geq 2}^{\infty} F_{nm}, \quad (4a)$$

$$F_{nm} \equiv a_{nm} [\rho(0)]^n [\rho_1^{\text{eff}}(T)]^m. \quad (4b)$$

We will discuss only terms with $m \leq 2$ and will carry $\rho_1^{\text{eff}}(T)$ to leading order in (kT/H_E) . Simple spin-wave theory gives

$$\rho(0) = \frac{1}{2N} \sum_k [(1 - \xi^2 \gamma_k^2)^{-1/2} - 1] \quad (5a)$$

$$\equiv \frac{1}{2N} \sum_k [\epsilon_k^{-1/2} - 1], \quad (5b)$$

so that approximately $\rho(0) \sim \xi^2/4z$. Thus Eq. (4) is in effect a $1/z$ expansion. Several authors⁶⁻⁸ have suggested that a $1/z$ expansion would be useful. In fact Wang, Shtrikman, and Callen⁷ have already pointed out that in the $1/S$ expansion $1/S$ always appears in the combination $1/zS$. From our analysis we see that the series consists of powers of $1/zS$ and $1/z$, or equivalently the coefficient of z^{-n} is an n th order polynomial in $1/S$. Our method seems to be the simplest way to actually construct terms in this series.

More precisely, we will group terms according to the number of factors γ_k over which averages are taken. Thus

$$\langle \gamma_k^2 \rangle \equiv N^{-1} \sum_k \gamma_k^2 = 1/z, \quad (6a)$$

$$\langle \gamma_k^4 \rangle \equiv N^{-1} \sum_k \gamma_k^4, \quad (6b)$$

$$\begin{aligned} \langle \gamma_k \gamma_{k'}, \gamma_{k-k'} \rangle &\equiv N^{-2} \sum_{kk'} \gamma_k \gamma_{k'} \gamma_{k-k'} \\ &= N^{-2} (\sum_k \gamma_k^2)^2 \end{aligned} \quad (6c)$$

are, respectively, of first, second, and second order in $1/z$. It is readily seen, however, that in counting powers of γ_k , factors occurring in combination with occupation numbers, n_k , should not be counted: e.g., $N^{-1} \sum_k (\gamma_k)^2 n_k$ is of the same order in $1/z$ as $N^{-1} \sum_k n_k$. In addition to occupation numbers and factors of γ_k , there also appear in the perturbative expansion factors l_k^2 , $l_k m_k$, and m_k^2 , where l_k and m_k are the coefficients in the canonical transformation from the a_k 's and b_k 's to the normal-mode operators. But these quantities can also be expanded in powers of γ_k :

$$l_k^2 = (1 + \epsilon_k)/2\epsilon_k = 1 + \frac{1}{4}\xi^2 \gamma_k^2 + \dots, \quad (7a)$$

$$l_k m_k = -\xi \gamma_k / 2\epsilon_k = -\xi \gamma_k / 2 + \dots, \quad (7b)$$

etc. Since we evaluate $\rho_1^{\text{eff}}(T)$ only to lowest or-

der in kT/H_E , we can set the excitation energy of all hole lines (which carry a factor n_k) equal to zero in the energy denominators. Then the energy denominators will consist of a sum of excitation energies which can also be expanded in powers of γ_k .

Accordingly the procedure is as follows: With each Feynman diagram associate the proper factor. Expand all momentum-dependent quantities in powers of γ_k . Collect together all terms with the same number of factors of γ_k to obtain a $1/z$ expansion of the form of Eq. (4). In so doing it is rather inconvenient to express the perturbation in terms of normal coordinates. Instead, as suggested previously,⁹ it is easier to work in the a, b representation using unperturbed propagators according to H_0 , so that

$$\begin{aligned} \langle a_k^\dagger b_{-k}^\dagger \rangle_0 &= \langle b_k^\dagger b_k \rangle_0 \\ &= n_k / \epsilon_k + (1 - \epsilon_k) / 2\epsilon_k, \end{aligned} \quad (8a)$$

$$\begin{aligned} \langle a_k^\dagger b_{-k}^\dagger \rangle_0 &= \langle a_k b_{-k} \rangle_0 \\ &= -(\xi \gamma_k / 2\epsilon_k)(1 + 2n_k), \end{aligned} \quad (8b)$$

where

$$n_k \equiv \{ \exp[\beta(H_E + H_A)\epsilon_k] - 1 \}^{-1}. \quad (9)$$

This leads to a slight revision in the usual^{10,11} rules for diagrammatic perturbation theory. In fact, since we set the energy of hole lines in the energy denominators to zero, we may construct these denominators as if all lines were particle lines. This simplification makes it very worthwhile to use the a, b representation.

We now give some results of our calculations. We have evaluated all contributions to the free energy with $n + m = 2$. To do this it is necessary to sum over all ladders made up of anisotropy vertices and at most one exchange vertex, because the latter carry a factor γ_k whereas the former do not. Hence we find

$$F_{02} = -\frac{H_E}{S} \sigma_1^2 - 4D\sigma_0^2 \left(1 - \frac{\xi}{2S} \right) \left(1 - \frac{D}{H_E + H_A} \right)^{-1}, \quad (10a)$$

$$F_{11} = -\frac{H_E \xi \sigma_1}{2zS} (\xi - 2) - \frac{D \xi^2 \sigma_0}{3Sz} \left[1 - \frac{2D}{3(H_E + H_A)} \right]^{-1} (6S - 2 - \xi^2), \quad (10b)$$

$$F_{20} = -\frac{H_E \xi^2 (\xi - 2)^2}{16z^2 S} - \frac{D \xi^4}{4z^2} \left[1 - \frac{D}{2(H_E + H_A)} \right]^{-1} \left(1 - \frac{1}{2S} \right), \quad (10c)$$

where $\sigma_1 = N^{-1} \sum_k (n_k / \epsilon_k) (1 - \xi \gamma_k^2)$. Note that for $S = \frac{1}{2}$, $\xi = 1$ and the results are independent of D . To the next order in $1/z$ we have only calculated terms independent of or linear in D , assuming $D \ll kT$:

$$F_{12} = -\frac{3\sigma_1^2 H_E}{4S^2 z} + \frac{D\sigma_0^2}{zS} \left(1 - \frac{1}{2S}\right) + \frac{4H_E \sigma_1^2}{zS^2}, \quad (11a)$$

$$F_{21} = -\frac{3}{2} D \langle \gamma^4 \rangle \sigma_0 \left(1 - \frac{1}{2S}\right) + \frac{D\sigma_0}{4z^2 S} \left(1 - \frac{1}{2S}\right) + \frac{H_E \sigma_1 \langle \gamma^4 \rangle}{8S} + \frac{H_E \sigma_1}{2z^2 S^2}, \quad (11b)$$

$$F_{30} = \frac{1}{64} \frac{H_E}{S^2 z^3} - \frac{3D}{8} \frac{\langle \gamma^4 \rangle}{z} \left(1 - \frac{1}{2S}\right) - \frac{H_E \langle \gamma^4 \rangle}{32S z}. \quad (11c)$$

Again the results are independent of D for spin $\frac{1}{2}$. As a further example of the preservation of spin kinematics we cite the lowest order evaluations for $D=0$:

$$\langle a_i^\dagger a_i^\dagger a_i a_i \rangle = 2(\sigma_0 + 1/4z)^2 (1 - 1/2S), \quad (12a)$$

$$\langle a_i^\dagger a_i^\dagger a_i^\dagger a_i a_i a_i \rangle = 6 \left(\sigma_0 + \frac{1}{4z}\right)^3 \left(1 - \frac{1}{2S}\right) \left(1 - \frac{1}{S}\right). \quad (12b)$$

If $(\sigma_0 + 1/4z)$ is replaced by $\langle a_i^\dagger a_i \rangle$, these results have the same form as for the ferromagnet.¹²

Finally we note that the spin-wave excitation energy can be obtained from our expressions for the free energy via¹³

$$E_k(T) = \delta F / \delta n_k, \quad (13)$$

which gives,¹⁴ for $D=0$,

$$\frac{E_k(T)}{H_E \epsilon_k} = 1 - \frac{\sigma_1}{S} + \frac{1}{4zS} - \frac{3\sigma_1}{4zS^2} + \frac{\langle \gamma^4 \rangle}{16S}, \quad (14)$$

with corrections of order σ_1/z^2 or $1/z^3$. Due to the approximations in $\rho_1^{\text{eff}}(T)$ this result is only valid for small wave vectors. It is clear that the corresponding expression for $D \neq 0$ would display no gap for spin $\frac{1}{2}$.

From this work we draw the following conclusions. For thermodynamic quantities the $1/z$ expansion, in contrast to the $1/S$ expansion, does preserve the spin kinematics and leads to rapidly convergent results for cubic lattices. Simple dynamical properties, like the spin-wave excitation energy at long wavelength, can also be calculated successfully by this method. The problem of calculating the energy width of spin waves and of obtaining bound states¹⁵ is more complicated and will be discussed elsewhere.

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¹⁴In Eq. (13) the derivative is with respect to the renormalized occupation numbers, whereas Eqs. (10) and (11) involve unperturbed occupation numbers. In terms of renormalized occupation numbers the formulas are the same except that the last term in Eqs. (11a) and (11b) are missing.

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